SURFACE 3D NANOSTRUCTURING BY TIGHTLY FOCUSED LASER PULSE: LAGRANGIAN CODES AND MOLECULAR DYNAMICS

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International Conference on Computer Simulation in Physics and beyond

September 6-10, 2015, Moscow, Russia

Physics <> Computer Simulations

- Laser-matter interaction

- Laser photon energy **E**/ W/ I τ_{las}

- Matter **metals** **semiconductors** dielectrics

- Geometry: *size of irradiated spot* – structure of a target

Photon energy

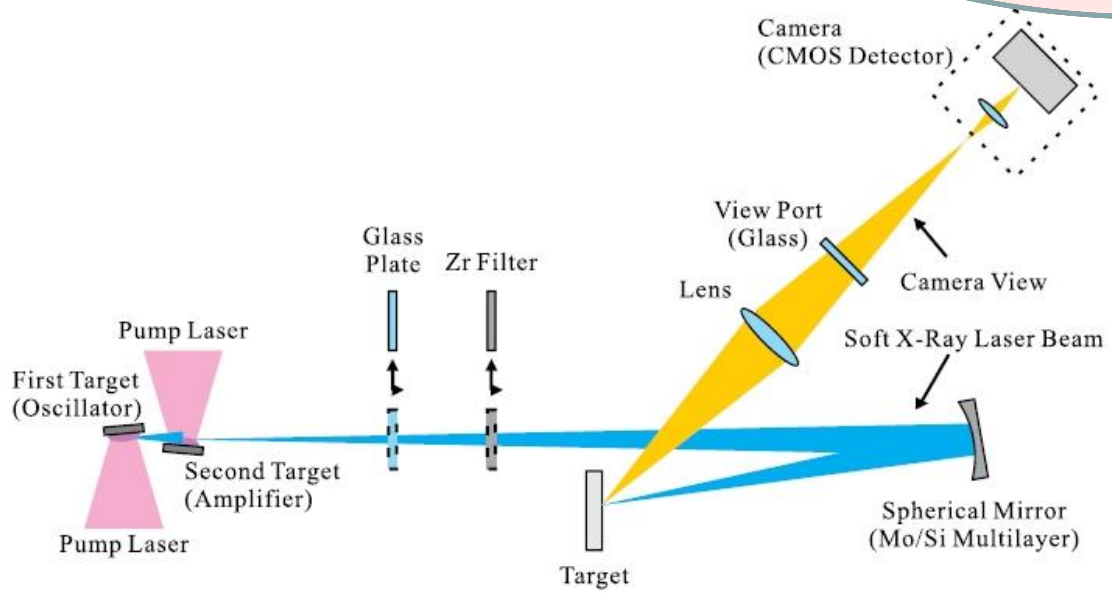
- From IR, optical to **EUV / soft X-ray – 10 keV**

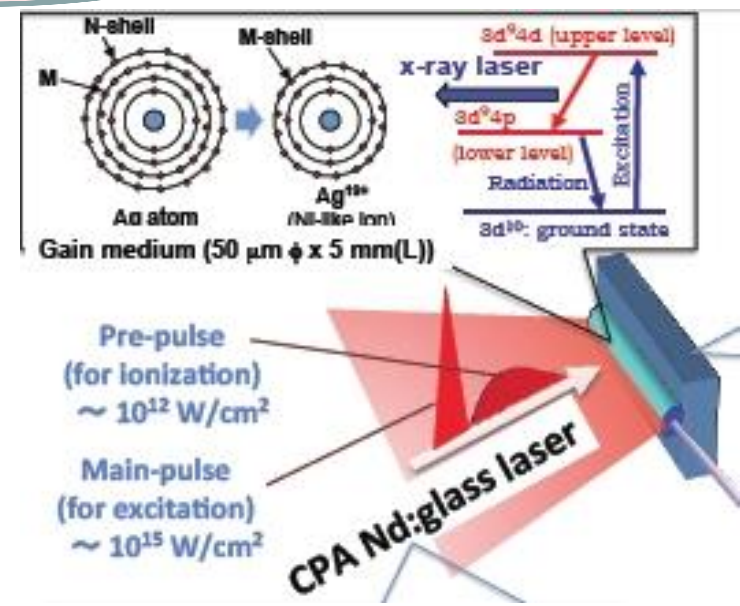
IR-optical lasers. Cr:forsterite (left) 1 eV and Ti:sapphire 1.5 eV.
Joint Inst.for High Temp. of RAS, Femtocenter, M.B. Agranat laboratory

Agranat et al., Appl.Surf.Sci.(2007); Anisimov et al., Appl.Phys.A (2008); Inogamov et al., JETP(2008); Appl.Surf.Sci.(2009); Appl.Phys.A(2010); Agranat et al., JETP Lett.(2010); Inogamov et al., Contrib. Plasma Phys.(2011); Ashitkov et al., JETP Lett.(2012); Inogamov et al., Contrib. Plasma Phys.(2013); J. Phys. Conf. Ser.(2014); Ashitkov et al., Quantum Electronics(2014); Inogamov et al., Engin.Failure Analysis(2015); Appl.Phys.B(2015); Ashitkov et al., Quantum Electronics(2015);

Photon energy

- From **IR, optical** to **EUV / soft X-ray – 10 keV**





Kansai Photon Science Institute, Japan Atomic Energy Agency:

Oscillator –Amplifier SXRL

Ag → Ag^{+19} Ni like ion
Far field image ~ 0.2 mrad
$\Delta\lambda/\lambda \sim 10^{-4}$

Faenov et al., Appl. Phys. Lett. (2009); Inogamov et al., Contr. Plasma Phys. (2009); Appl. Phys. A (2010); Ishino et al., J. Appl. Phys. (2011); Inogamov et al., Contr. Plasma Phys.(2011a; 2011b); J. Opt. Technol. (2011); J. Phys. Conf. Ser. (2014a; 2014b); Ishino et al., J. Appl. Phys. (2014); Inogamov et al., Engin. Failure Analysis (2015); Appl. Phys. B (2015);

Photon energy

- From **IR, optical** to **EUV / soft X-ray – 10 keV**

X-FEL SACLA (shown, http://xfel.riken.jp)
LCLS = Linac Coherent Light Source at SLAC
Europian XFEL/DESY

Ablation of dielectrics and metals by EUV-FEL at Spring-8=the work done few years ago
Current work is: pump-probe with the subnanosecond pump and the XFEL probe

Ablation of dielectrics and metals by EUV-FEL at Spring-8= the work done few years ago

- EUV-FEL photon energy 20 eV

Contrib. Plasma Phys. **51**, No. 5, 419 – 426 (2011) / **DOI** 10.1002/ctpp.2011100013

Two-Temperature Warm Dense Matter Produced by Ultrashort Extreme Vacuum Ultraviolet-Free Electron Laser (EUV-FEL) Pulse

N. A. Inogamov*[1], A. Ya. Faenov[2,3,7], V. V. Zhakhovsky[2,4], T. A. Pikuz[2,3,7], I. Yu. Skobelev[2], Yu. V. Petrov[1], V. A. Khokhlov[1], V. V. Shepelev[5], S. I. Anisimov[1], V. E. Fortov[2], Y. Fukuda[3,7], M. Kando[3], T. Kawachi[3], M. Nagasono[7], H. Ohashi[7,8], M. Yabashi[7,8], K. Tono[7], Y. Senda[8], T. Togashi[7,8], and T. Ishikawa[7]

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[2] Joint Institute for High Temperatures, Russian Academy of Sciences, Moscow 125412, Russia
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Physics <> Computer Simulations

- <u>Laser-matter interaction</u>

- Laser   photon energy   **E**/ W/ I τ_{las}

- Matter…

Ti:sapp ~ 1 eV

SACLA XFEL up to ~ 10^4 eV

Physics <> Computer Simulations

- <u>Laser-matter interaction</u>

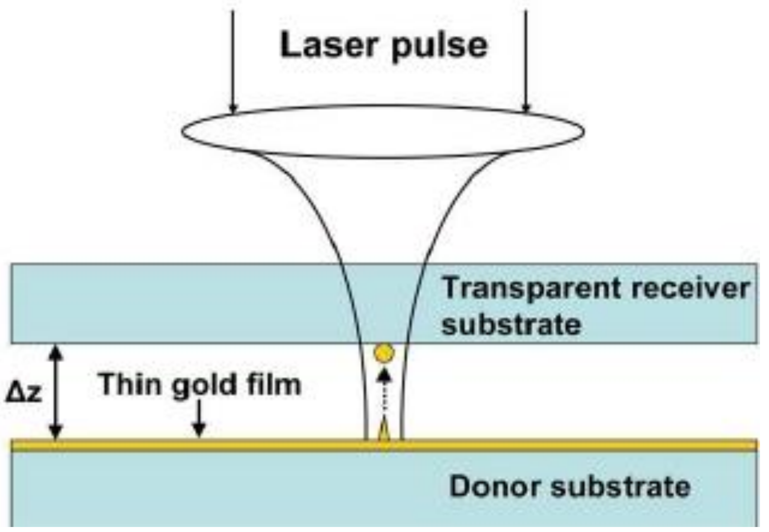
- Laser photon energy **E**/ W/ I τ_{las}

- Super powerful machines NIF & LMJ

- Petawatt lasers+spot 4*4 um^2 $\rightarrow$ $I \sim 10^{21}$ W/cm^2
  – at 10^{19} electron oscillation energy is $\sim m_e c^2$

Physics <> Computer Simulations

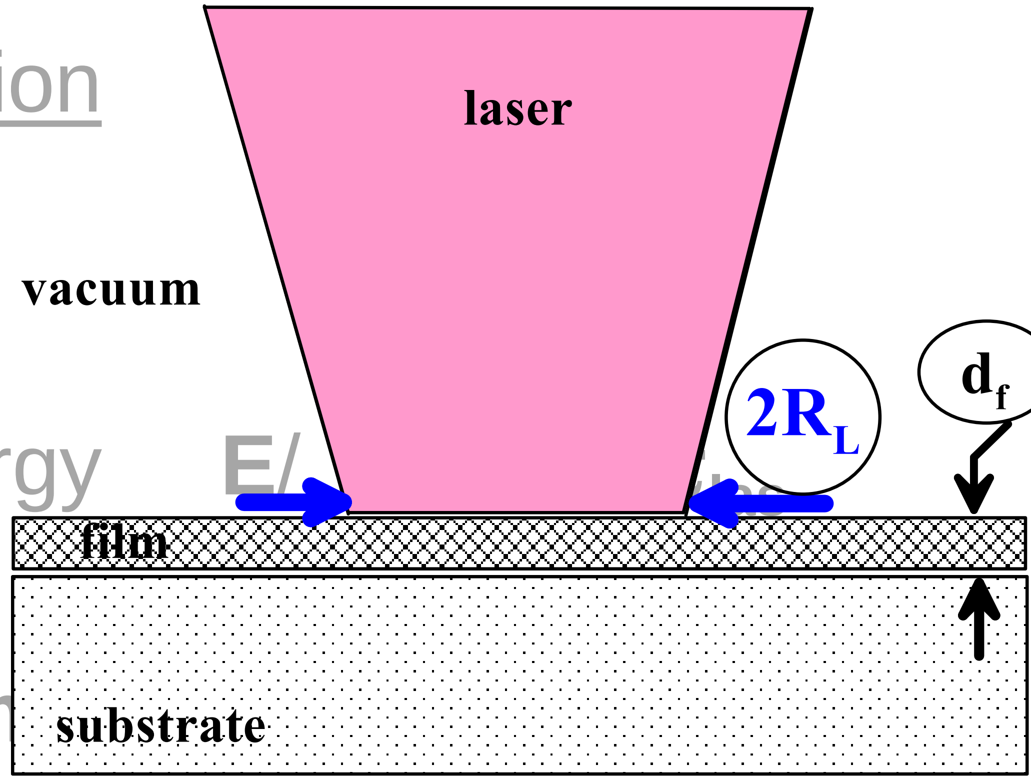
- Our physics: Below we consider the case of moderate intensities F~ 0.1-100 J/cm^2
- It is important for technological applications
- LIFT, laser printing, nanoplasmonics, SERS, nanoparticle formation



Kuznetsov et al., Opt.Express (2009).

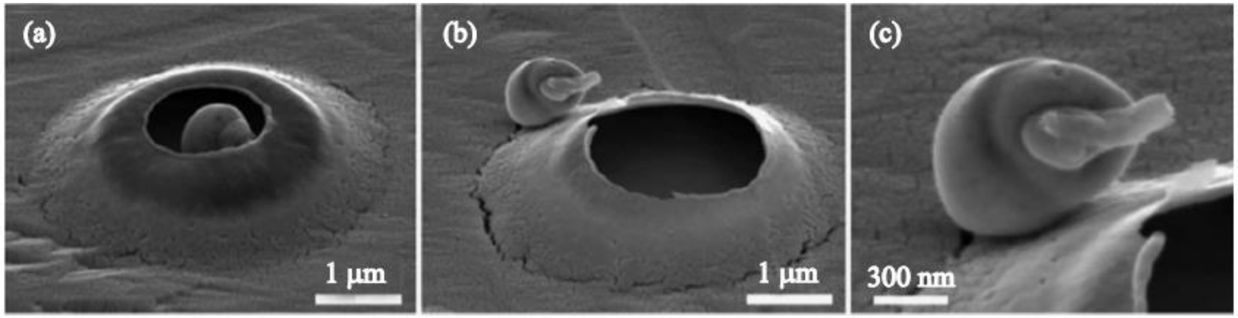
Physics <> Computer Simulations

- Laser-matter interaction

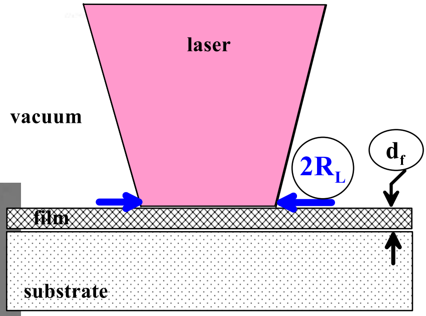


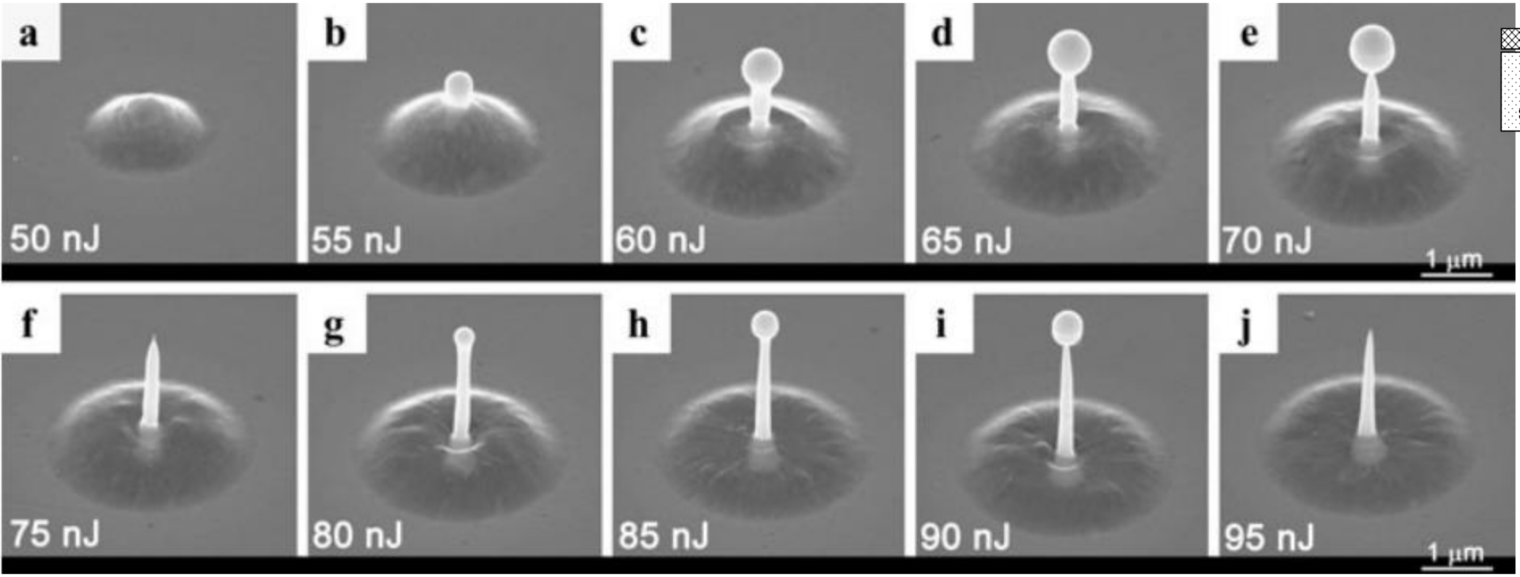
- Laser photon energy E/
- Matter **metals** **sem**
- **Geometry**: ***size*** *of irradiated spot* – **structure** of a target

Tightly focused case: $R_L \sim \lambda$



SEM images: Emel'yanov et al., JETP Lett. (2014)





Kuznetsov *et al*., Appl. Phys. A (2012)

Physics <> **Computer Simulations**

- DFT, QMD
- Band structure, wave functions
- Kubo-Greenwood, **electron transport**
- VASP (https://www.**vasp**.at/)
- ABINIT (www.abinit.org/)
- Elk (http://elk.sourceforge.net/)
- DMOL3 (http://accelrys.com/)
- **EAM** interatomic potentials **(force matching vs. stress matching)**
- **Electron additions** into wide-range EoS

Physics <> Computer Simulations

- **electron transport**
- **EAM** interatomic potentials
- **Electron additions** into wide-range EoS

- Then we run two-temperature **hydrodynamic codes**
- LAMMPS Molecular Dynamics Simulator
- **MPD**[3]: material particle
- dynamical
- domain
- decomposition

MPD^3

A New Dynamical Domain Decomposition Method for Parallel Molecular Dynamics Simulation

V. Zhakhovskii[1], K. Nishihara[1], Y. Fukuda[1], S. Shimojo[2], T. Akiyama[2], S. Miyanaga[2], H. Sone[3], H. Kobayashi[3], E. Ito[3], Y. Seo[4], M. Tamura[4], and Y. Ueshima[5]

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[4]*NEC Corporation, Japan*
[5]*Advanced Photon Research Center, JAERI, Japan*

Intern. Symp. On CCGrid2005. pp. 848-854, vol. 2 (2005)

MPD^3

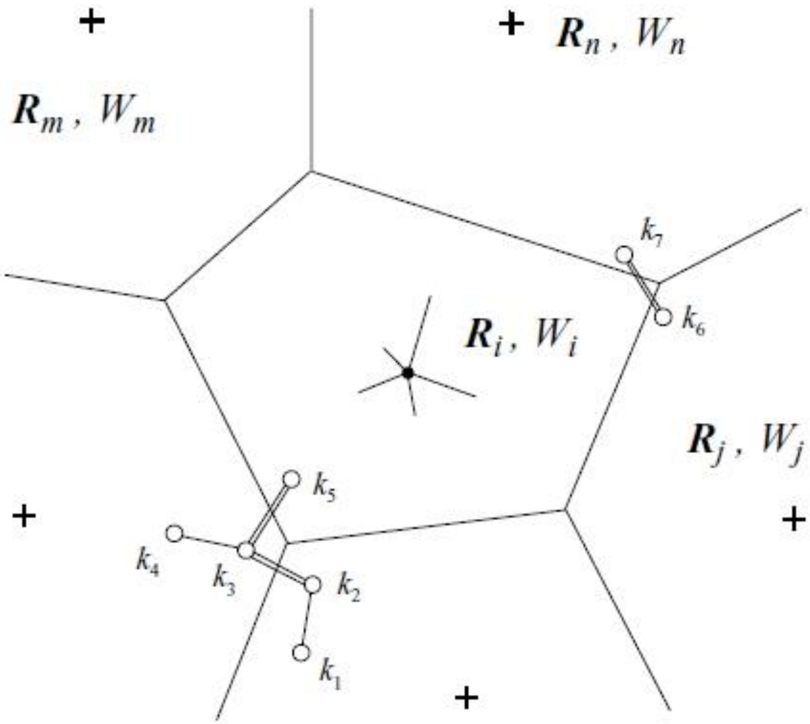


Fig. 2. **Two dimensional Voronoi domain decompositions. Crosses denote centers of subdomains called as material particles. Circles and k indices mark simulated atomic particles, like ions, atoms and molecules.**

MPD³

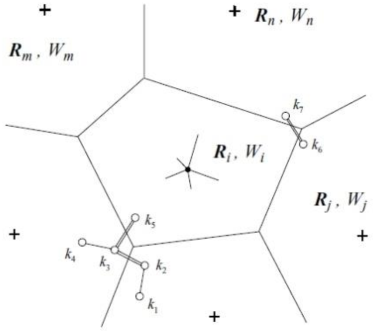


Fig. 2. **Two dimensional Voronoi domain decompositions. Crosses denote centers of subdomains called as material particles. Circles and k indices mark simulated atomic particles, like ions, atoms and molecules.**

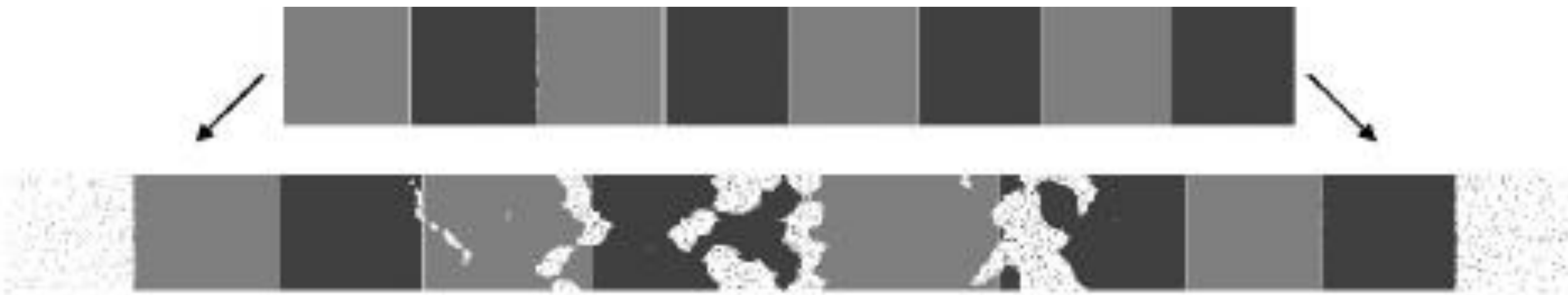
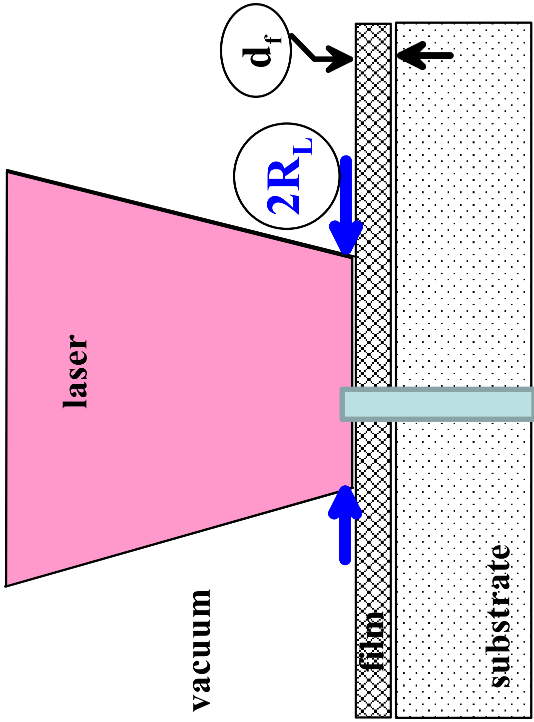
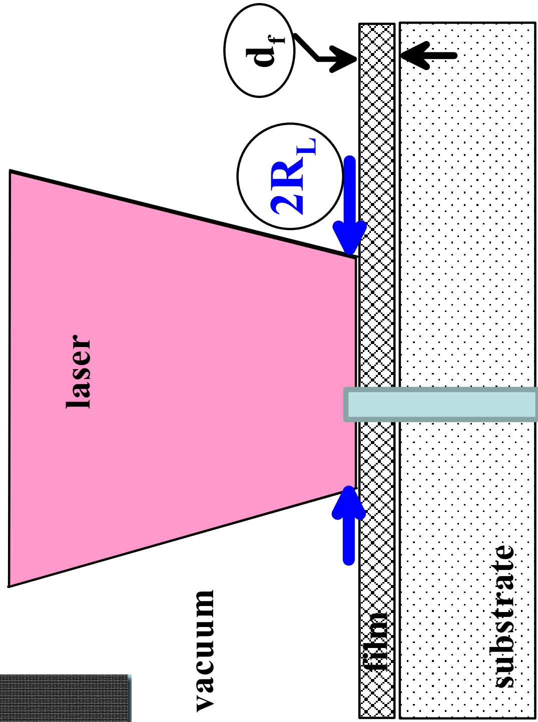


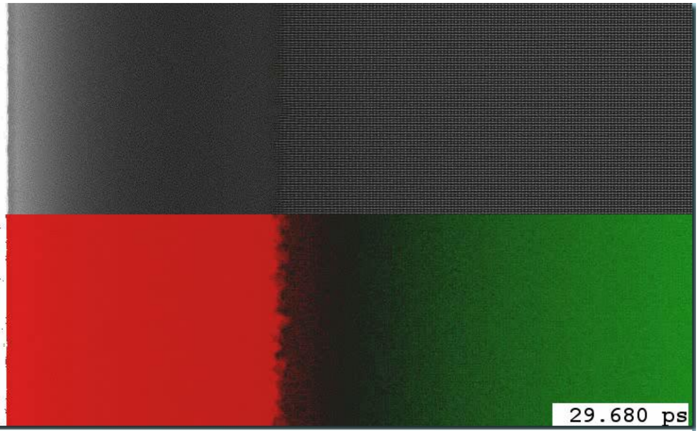
Fig. 4. Snapshots of formation of central and peripheral cracks taken from [6]. On top the initial 1D decomposition among 8 identical SX-5 CPUs. On bottom the final structure of MPD^3 . The load balance was perfect during all simulation.

Homogeneous irradiation: large R_L



Homogeneous irradiation: large R_L and bulk target

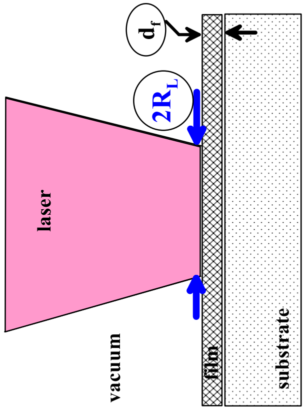




Ablation of frontal part of gold film at absorbed laser fluence 295 mJ/cm^2.
Map of density on the top. Map of local atomic order on the bottom.

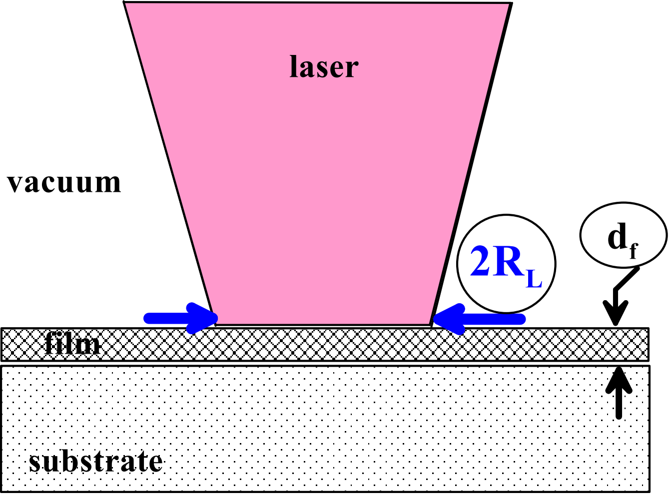
Brian J. Demaske, Vasily V. Zhakhovsky, Nail A. Inogamov, Ivan I. Oleynik

Rear-side spallation

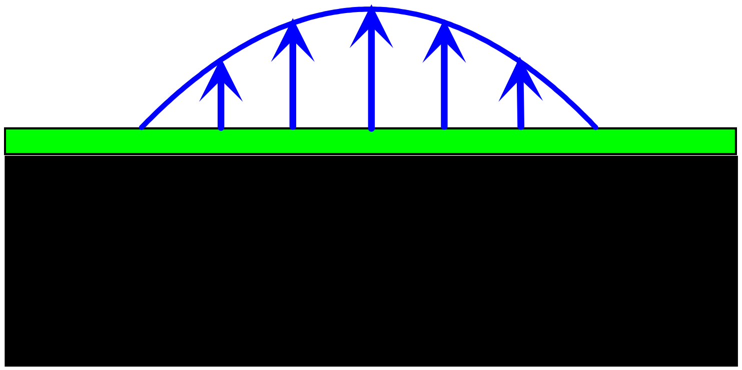


[redacted]

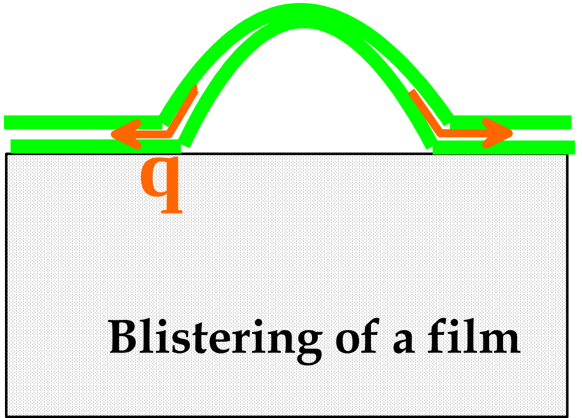
Small spot, thin film

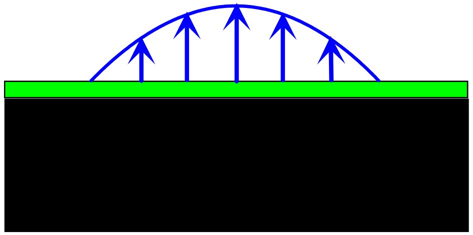


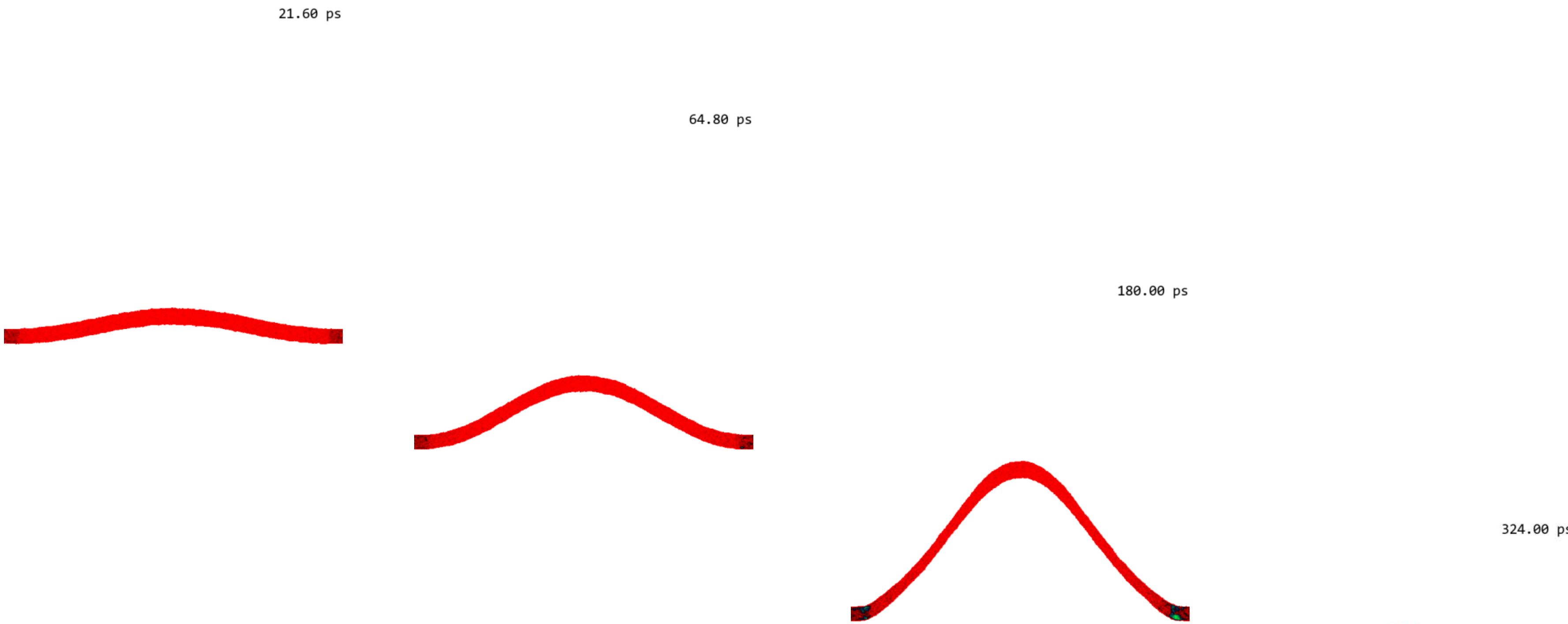
Finite size of a beam, maximum of fluence at the axis

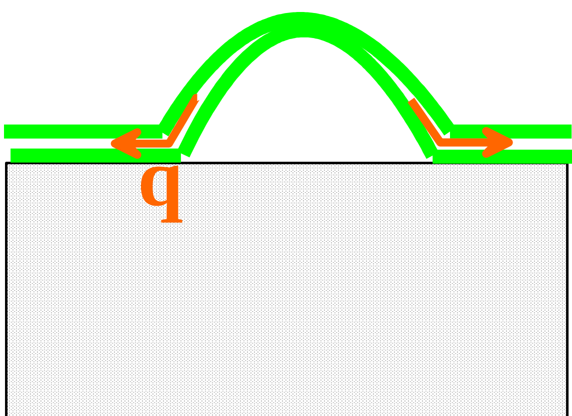


Velocity distribution created by the beam



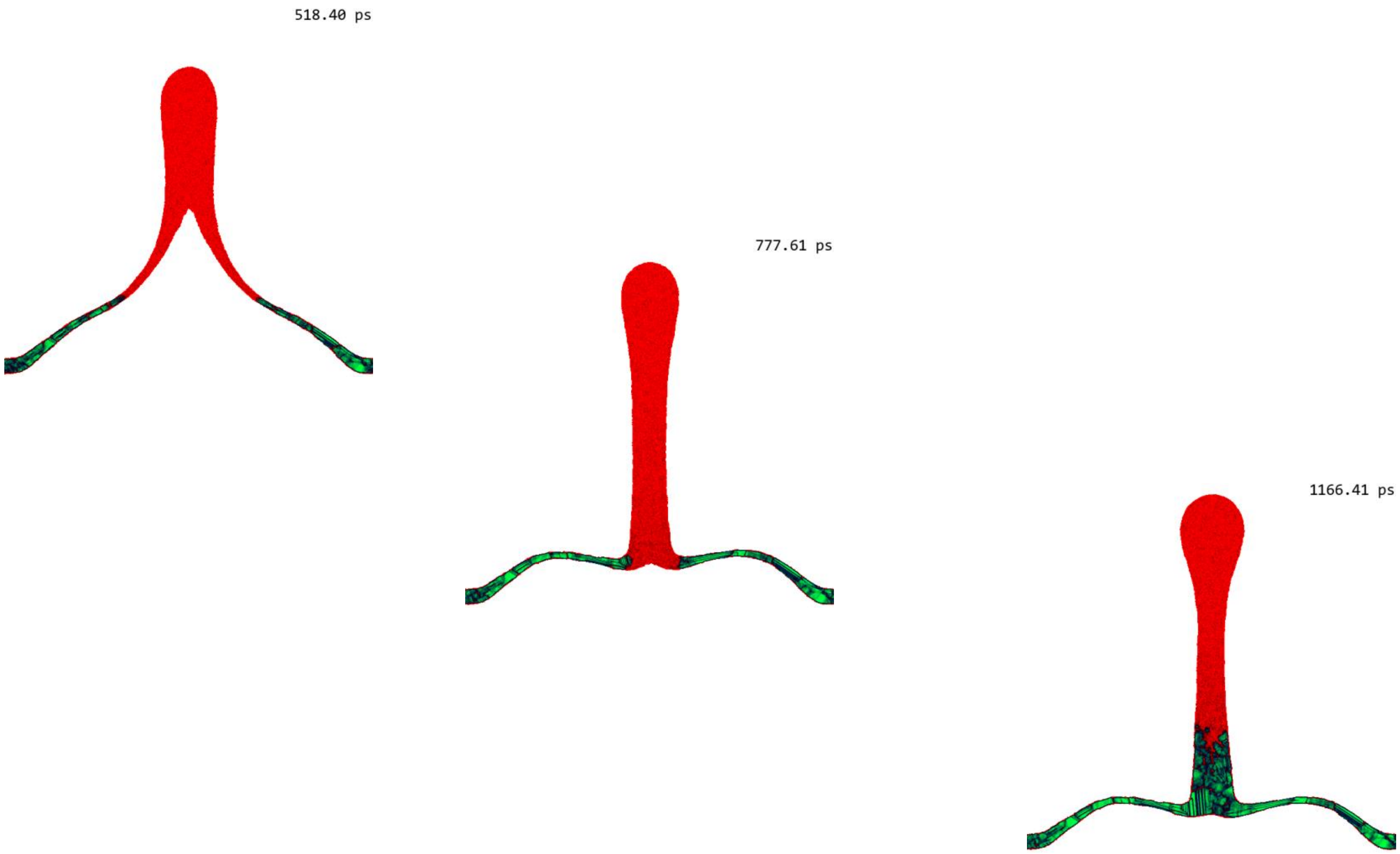






Molecular Dynamics-Monte-Carlo (MD-MC) cooling:
Red is molten gold, green is solid

Formation of a jet

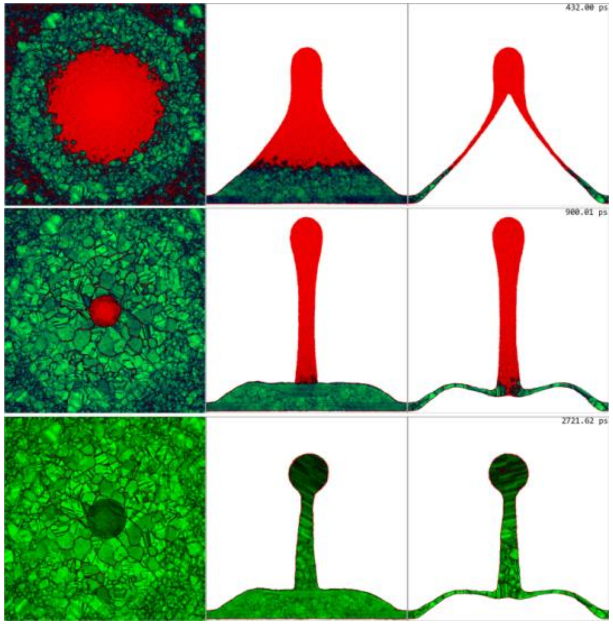


Explanation of jetting: flow toward the axis

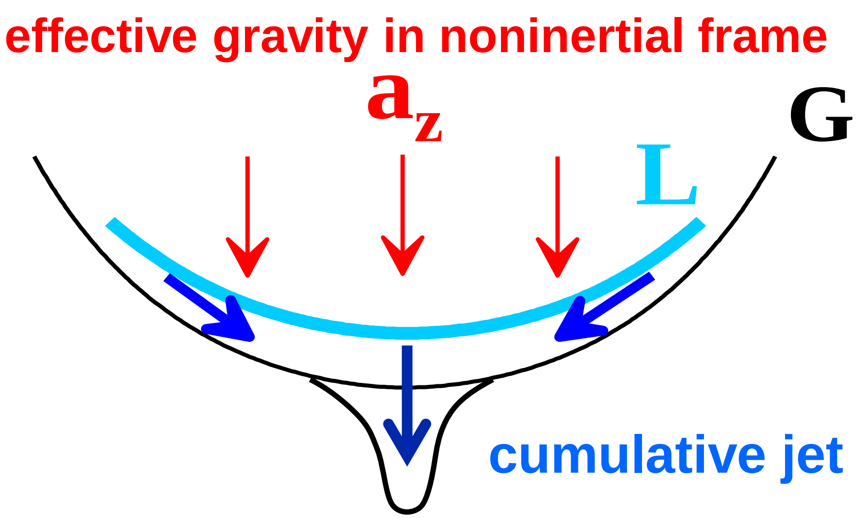
Laser heating → **Thermal expansion**

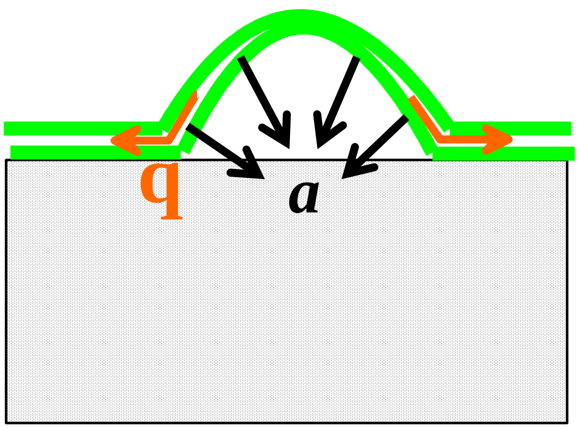
Thermal expansion versus

Deceleration by surface tension



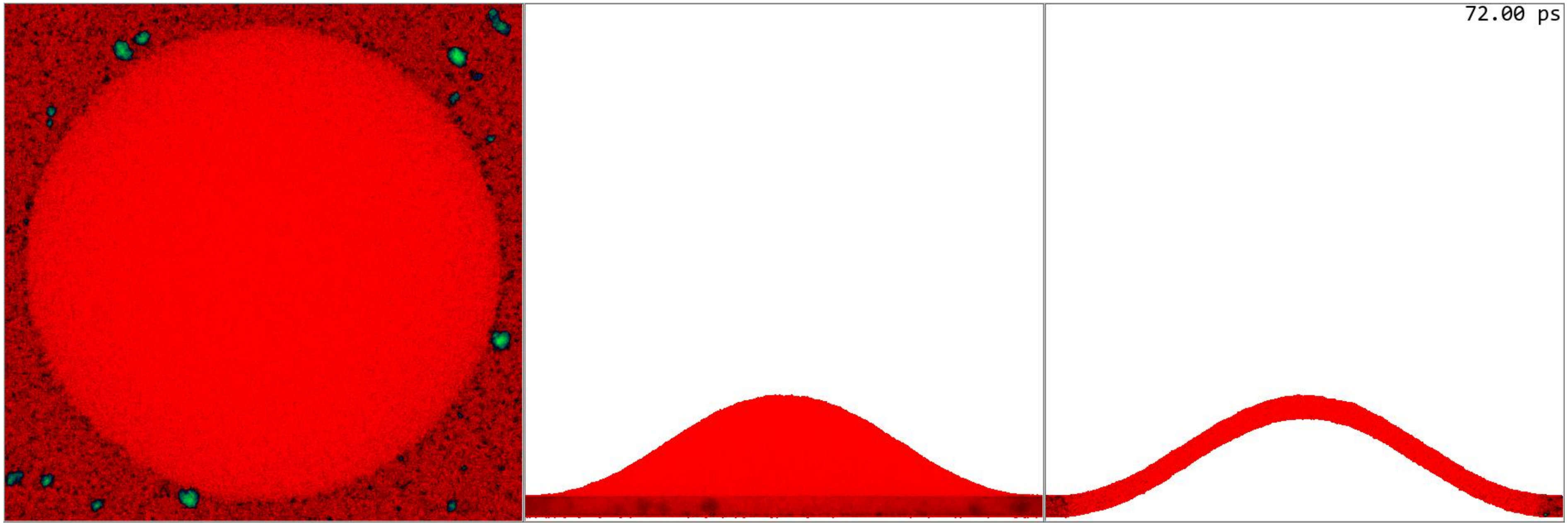
Surface tension → vertical deceleration + radial acceleration, which drives material flow toward axis → near axis accumulation of material forms an axial cumulative jet





Results of MD simulation

Formation and solidification of a jet in the apex of the nanobump

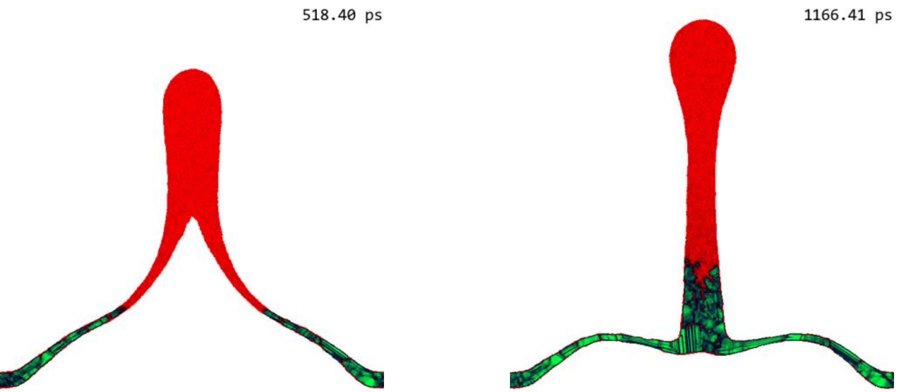


Gold film, combined MC-MD simulation

Red is molten gold.
Green is solidified gold.

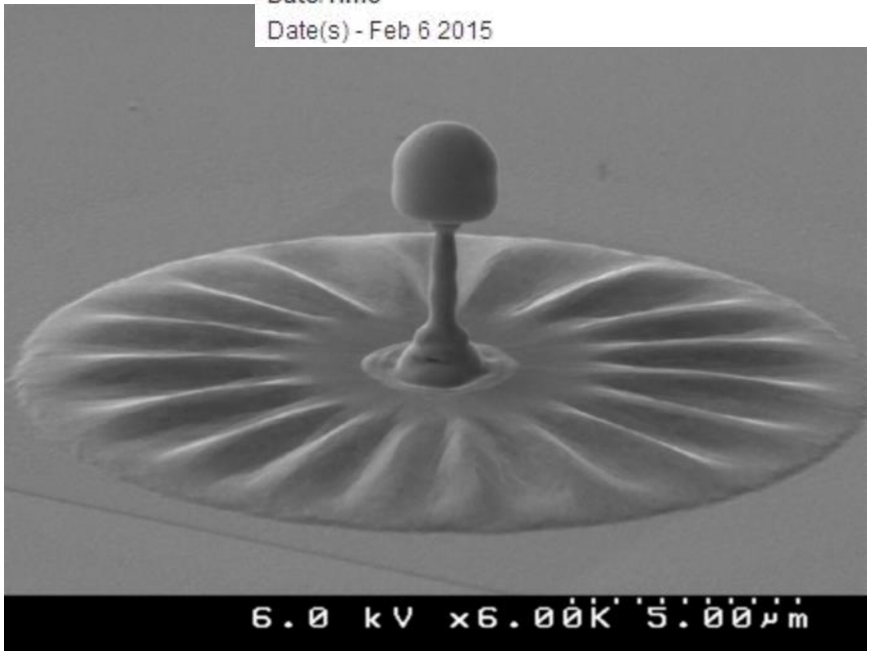
N.A. Inogamov et al, JETP Lett. 100 p. 4 (2014)
N.A. Inogamov et al, JETP 120, p. 15 (2015)

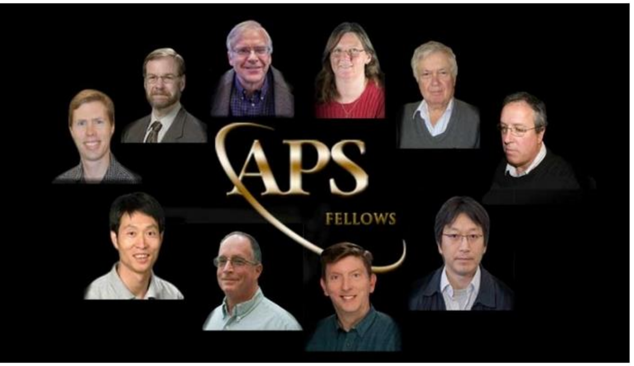
Freezing of the skirt
Motion down of the solidified skirt
Folding of the surface excess =
this is our explanation how the radial ripples appear



Mike Armstrong (SIMES Seminar)

Date/Time
Date(s) - Feb 6 2015





The American Physical Society named 10 Lawrence Livermore researchers as 2014 fellows. Top row from left, Michael Armstrong, Chris Barty, Ray Beach, Debbie Callahan, Tony Gonis and Frederic Hartmann. Bottom row from left, Yinmin "Morris" Wang, James Tobin, Robert Rudd and Nobuhiko Izumi. (Download Image)

Ten Lawrence Livermore National Laboratory researchers named 2014 APS fellows

https://simes.stanford.edu/events/mike-armstrong-simes-semina

Conclusion

- Experiments on laser-matter interaction often give us only final results
- Computer simulations are necessary to understand the sequence of events that lead to these final results
- Physics is cumbersome therefore several codes complementary to each other are used: DFT, QMD → EAM → MD

Thank you for your attention